Phosphoramidic acid, dimethyl-, dimethyl ester

597-07-9 DTXSID20208405	

Model Performance

Model	Data	

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: -0.335

Global applicability domain: Inside

Local applicability domain index: 4.00e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found

2-(2-Methyl-2-imidazolin-1-

yl)ethanol

Measured: 0.04 Predicted: -0.266

Image not found

Trimethyl phosphate

Measured: -0.650 Predicted: -0.414

Image not found

Tetramethylurea

Measured: 0.19 Predicted: 2.74e-01

Image not found

2,4(1H,3H)-Pyrimidinedione, 1,3-

dimethyl-

Measured: -0.540 Predicted: -0.553